

Quantum simulator for many-body electron–electron Coulomb interaction with ion traps

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We propose an analog quantum simulator that uses ion traps to realize the many-body electron–electron Coulomb interaction of an electron gas. This proposal maps a system that is difficult to solve and control to an experimentally-feasible setup that can be realized with current technologies. Using a dilatation transform, we show that ion traps can efficiently simulate electronic Coulomb interactions. No complexity overhead is added if only the energy spectrum is desired, and only a simple unitary transform is needed on the initial state otherwise. The runtime of the simulation is found to be much shorter than the timescale of the corresponding electronic system, minimizing susceptibility of the proposed quantum simulator to external noise and decoherence. This proposal works in any number of dimensions, and could be used to simulate different topological phases of electrons in graphene-like structures, by using ions trapped in honeycomb lattices.

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Introduction.— Many-body interactions are fundamental to understanding a variety of interesting phenomena. Quantum many-body problems are notoriously difficult to solve for the full energy spectrum, and are even more problematic for dynamical properties. Few realistic exactly-solvable models exist, necessitating approximations that typically are valid only in some regions of the parameter space. The root of this difficulty is that the Hilbert space grows exponentially as the number of quantum particles increases [1], so on a classical computer the resources and time required to solve a problem exhibit a corresponding exponential growth. Some powerful numerical tools such as quantum Monte Carlo methods and the density matrix renormalization group have had some success for some systems, but the complexity involved prevents an efficient numerical study of many other interesting problems, especially for quantum dynamics and higher-dimension systems.

A powerful alternative to calculation is *quantum simulation* [1–3]. A universal quantum computer has not yet been realized but quantum simulations of specific systems have enjoyed considerable success, aided by experimental advances such as the realization of high-fidelity quantum gates and increasingly precise measurement [4, 5]. They have been used to study quantum phase transitions [6], open quantum systems [7], and pairing Hamiltonians [8], to name just a few applications. Quantum simulators follow the laws of quantum mechanics, with an exponentially-growing computing capability [1, 2] that can match the exponential growth of problem size with particle number. The idea to simulate one quantum system with another has been proven [9] to be efficient, at least for any many-body system having only few-body particle correlations.

A quantum simulator works by designing a custom Hamiltonian H_s so that the evolution operator $U = \hat{T} \exp[-i \int_0^t H_s d\tau]$ behaves like the physical system one wishes to simulate. Then

a precise measurement at the end of the time evolution gives the physical quantity of interest. A useful quantum simulator requires high-fidelity Hamiltonian engineering and initialization, and precise measurement. A number of systems have been realized experimentally to implement the quantum simulation task, including ion traps, ultracold atoms in optical lattices, NMR nuclear spins, and superconducting qubits.

Many-body electron–electron (e–e) Coulomb interactions play a critical role in many important phenomena such as the fractional quantum Hall effect [10, 11] and high T_c superconductors [12]. Dealing with the mutual Coulomb interactions between all the electrons is daunting but essential to a deep understanding of such systems. In this Letter, we propose to use quantum simulations to obtain the properties of systems exhibiting many-body e–e Coulomb interactions. The quantum simulator may be realized using an ion trap [2, 13, 14]. Control methods for ion traps may be implemented with current technologies [4, 5] and they have been used widely in quantum simulation and quantum information tasks [15], with applications in areas such as quantum chemistry [16] and mass spectrometry [17].

Electrons in the physical system to be emulated and ions in the trap carry different masses and charges, so a direct simulation is not possible. However, we have employed a dilatation transform to establish an explicit mapping between the simulator on one timescale and the interacting electrons on a different timescale. Therefore, the ion trap at rescaled times can be used to simulate the e–e Coulomb interactions at physical times. To read out the results, we propose imaging of the ions to record their positions, which then have a direct mapping to the positions of the interacting electrons. Remarkably, if only the energy spectrum is desired the unitarity of the dilatation transform implies that it will not alter the spectrum so it is not necessary to generate the transform physically.

This proposal is dimensionality-agnostic. For example, it

could be employed for simulating the behavior of 2D electron gases. For charged particles confined in 2D, some interesting phenomenon can arise, such as various quantum Hall effects [10, 11]. Moreover, by loading the ions in honeycomb lattices, one could also realize different topological phases characterizing the behavior of electron in graphene-like structures [32]. The ion trap simulator allows for a study of the finite-size boundary effects for the interacting electrons, where bound states are possible. As a concrete example of this proposal, we shall illustrate the experimental setup of the quantum simulation by using calcium ions carrying one positive charge.

The interacting electron gas.— An interacting electron gas can be described by the Hamiltonian ($\hbar \equiv 1$) [18]

$$H_{\text{eg}} = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m_e} + \sum_{i<j}^N \frac{e^2}{|\mathbf{q}_i - \mathbf{q}_j|}, \quad (1)$$

where m_e is the electron mass and \mathbf{p}_i and \mathbf{q}_i are the momentum and position operators, respectively, for the i -th electron. The first term represents the kinetic energy and the second term represents the potential energy resulting from mutual Coulomb interactions among the electrons. Because of the many-body nature of the problem, the Hilbert space grows exponentially with electron number, making an exact solution of the Schrödinger equation difficult. Although in some cases it may be possible to consider only the average effect of the electrons (mean field approximations), a complete description requires accounting for the interaction between all electrons.

Traditionally, perturbation theory approximations or numerical tools have been used to tackle this problem, with mixed success. In this Letter, we take a fundamentally different approach: we propose an experimentally-feasible quantum simulator that can faithfully represent the Coulomb interaction between the electrons, thus bypassing cumbersome calculations.

Ion-trap simulator.— Typically quantum simulation consists of three stages: (1) preparation of an initial state, (2) time evolution under a specifically-engineered Hamiltonian, and (3) readout of the result, which can be achieved through quantum phase estimation procedures or measurement. Assuming the quantum simulator to be well-controlled experimentally, the most critical task is to design a Hamiltonian of the quantum simulator leading to the required propagator, so that a map exists between the initial and final states of the simulator and those of the system under consideration [2]. Ion traps are widely-used and experimentally well-controlled systems, with the ions either localized or undergoing axial and cyclotron motions as in Penning traps [19]. Since the fermionic ions exhibit mutual Coulomb interaction, an ion trap loaded with identical ions may be a good candidate for the simulation of e-e Coulomb interactions.

To simulate the electron gas, we propose an analogue quantum simulator using an ion trap with N identical ions interacting by Coulomb interactions, as illustrated schematically in

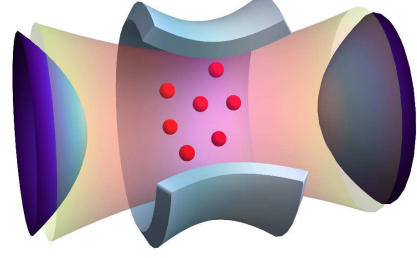


FIG. 1: (Color online) Schematic representation of the ion-trap simulator for Coulomb interactions: N identical ions, mutually interacting via the Coulomb force.

Fig. 1. The Hamiltonian is given by

$$H_s = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m_{\text{ion}}} + \sum_{i<j}^N \frac{Q^2 e^2}{|\mathbf{q}_i - \mathbf{q}_j|}, \quad (2)$$

where m_{ion} is the mass of the ion and Q is the degree of ionization. This Hamiltonian is formally similar to Eq. (1) but there are two significant differences: (1) The ion to electron mass ratio is of order $10^4 - 10^5$ for ions such as $^9\text{Be}^+$ or $^{111}\text{Cd}^+$ commonly used in traps, and Q may be greater than 1. Since the kinetic term and the Coulomb interaction terms do not commute, these disparities rule out direct use of the ion trap as an analog simulator for this problem. For the ion trap to faithfully simulate the e-e Coulomb interaction, an explicit mapping between the two systems is required. We shall now show that this can be achieved by the introduction of a scaled evolutionary time for the simulator.

Dilatation operator. Let us consider the (unitary) dilatation operator [20]

$$S(\mathbf{r}) = \exp \left[\sum_{j=1}^N \frac{ir_j}{2} (\mathbf{q}_j \cdot \mathbf{p}_j + \mathbf{p}_j \cdot \mathbf{q}_j) \right], \quad (3)$$

where $\mathbf{r} = (r_1, \dots, r_N)$, with r_k being a real dilatation parameter for the k th particle. Using the Baker–Campbell–Hausdorff formula

$$\exp[\alpha A] B \exp[-\alpha A] = B + \sum_{m=1}^{\infty} \frac{\alpha^m}{m!} [{}_m A, B] \quad (4)$$

where $[{}_m A, B] = [A, [{}_{m-1} A, B]]$ and $[{}_1 A, B] = [A, B]$ is the commutator, one finds that for the k th particle the position and momentum operators transform as

$$S^\dagger(\mathbf{r}) \mathbf{q}_k S(\mathbf{r}) = \exp(-r_k) \mathbf{q}_k, \quad S^\dagger(\mathbf{r}) \mathbf{p}_k S(\mathbf{r}) = \exp(r_k) \mathbf{p}_k. \quad (5)$$

Thus the dilatation transform scales the momentum and position terms differently, allowing the ratio between the two terms in the Hamiltonian (2) to be tuned.

We take $r_k \equiv r$ for $k = 1, \dots, N$ and denote the corresponding dilatation transform as $S(r)$. Because $S(r)$ is unitary,

$$S^\dagger(r) f_k(\mathbf{p}_k, \mathbf{q}_k) S(r) = f_k(\exp(r)\mathbf{p}_k, \exp(-r)\mathbf{q}_k)$$

for any operator functions f_k and

$$\tilde{H}_s \equiv S^\dagger(r) H_s S(r) = \exp(r) Q^2 \left[\sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m_{\text{eff}}} + \sum_{i<j}^N \frac{e^2}{|\mathbf{q}_i - \mathbf{q}_j|} \right], \quad (6)$$

where $m_{\text{eff}} = \exp(-r) Q^2 m_{\text{ion}}$ represents the effective mass after the dilatation. Then, by requiring $m_{\text{eff}} = m_e$, one recovers exactly the e-e Hamiltonian in Eq. (1). This relation fixes the dilatation parameter r and the scaled runtime $\tilde{t} = t/(\exp(r) Q^2)$, so that the evolution operator is

$$U(t) = \exp(-iH_{\text{eg}}t) = S^\dagger(r) \mathcal{U}(\tilde{t}) S(r), \quad \mathcal{U}(\tilde{t}) = \exp(-iH_s \tilde{t}). \quad (7)$$

This establishes a one-to-one mapping between the initial state $|\psi(0)\rangle$ of the interacting electrons and the initial state $|\phi(0)\rangle$ of the ion-trap quantum simulator, as well as between the corresponding final states $|\psi(t_f)\rangle$ and $|\phi(\tilde{t}_f)\rangle$, so that quantum simulation of the e-e Coulomb interactions using ion traps is possible.

Physically the map is a rotation described by the dilatation operator and a corresponding rescaling of time for the propagator. The dilatation parameter and the new time scale are determined solely by the mass ratio between the ion and electron, and the degree of ionization. As a bonus, since the mass of the electron is much less than that of the ions and $Q \geq 1$, we have $Q^2 \exp(r) \gg 1$. Therefore, to simulate the propagator $U(t)$ the simulator runtime \tilde{t} is much less than the physical runtime t . This efficiency is particularly beneficial since shorter runtimes decrease the susceptibility of the quantum simulator to external noise and decoherence. When we are interested in boundary effects or need to take into consideration the finite size nature of the simulator, the dilatation parameter also dictates the mapping between the boundaries of the electron gas and the ion trap size. For example, with a hard wall boundary of width w for the electron gas, the dilatation transform will map that to a hard wall boundary of width $\exp(-r)w$ for the ion trap. A similar scaling would apply to any external potential (as in the case of an honeycomb lattice), namely $V_s(\mathbf{q}) = Q^2 \exp(r) V_{\text{ext}}(\exp(r)\mathbf{q})$, where V_s and V_{ext} are the potentials for the ion-trap simulator and electron gas, respectively.

Readout. Results may be read out using an imaging technique to measure the position of the ions [21] in the trap and build up a history of the position over time. Assume that one prepares an arbitrary initial state of the simulator as $|\phi(0)\rangle = \int c_v |v\rangle$, where $|v\rangle$ labels the eigenvector with an eigenvalue of E_v . Then, a position measurement would return

$$\begin{aligned} \langle n(\mathbf{q}) \rangle &= \int dv dv' c_v^* c_{v'} \exp[i(E_v - E_{v'})t] \langle v | n(\mathbf{q}) | v' \rangle \\ &\equiv \int dv dv' F(v, v') \exp[i(E_v - E_{v'})t], \end{aligned}$$

where n is the density of state at position \mathbf{q} . The dilatation transformation is unitary, so that $U(t)$ and $\mathcal{U}(\tilde{t})$ have the *same spectrum*, which can be extracted by means of a simple Fourier transformation [8],

$$\bar{S}(\omega) = \int dv dv' \tilde{F}(v, v') \delta[\omega - (E_v - E_{v'})]$$

with the sharpness of the delta function being related to the sampling frequency of the measurements.

In principle, if one would like to simulate the dynamical evolution of a precise electronic initial state $|\psi(0)\rangle$, one should prepare the corresponding initial state of the simulator as $|\phi(0)\rangle = S(r)|\psi(0)\rangle$. This could be achieved by propagating the initial state $|\psi(0)\rangle$ using the Hamiltonian

$$H' = -\frac{1}{2} \sum_{j=1}^N (\mathbf{q}_j \cdot \mathbf{p}_j + \mathbf{p}_j \cdot \mathbf{q}_j) \quad (8)$$

for a time duration of r , according to Eq. (3). We then let the state propagate for a duration of t , followed by an inverse propagation of (8). Then, a measurement of the ions would give expectation values for the electron gas according to

$$\langle \phi(0) | \mathcal{U}^\dagger(\tilde{t}) O \mathcal{U}(\tilde{t}) | \phi(0) \rangle = \langle \psi(t) | O | \psi(t) \rangle,$$

where O is the observable under consideration and $\mathcal{U}(\tilde{t}) = S(r) U(t) S^\dagger(r)$.

We also envisage a more general way to obtain the spectrum, through the quantum phase estimation algorithm [22, 23]. This would require the coupling of the simulator to a quantum circuit capable of generating a controlled-U operation that takes a qubit state as control and applies the unitary operation on the wave function only if the control qubit is in the $|1\rangle$ state. For an estimated phase of n -bit precision, one needs n Hadamard gates to transform the n ancillary qubits from $|0\rangle$ to $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$. Denoting the controlled-U operation as

$$K_j = |1\rangle\langle 1|_j \mathcal{U}^{2^{j-1}}(\tilde{t}) + |0\rangle\langle 0|_j \mathbb{1},$$

for the j th qubit $|q_j\rangle = c_0|0\rangle_j + c_1|1\rangle_j$, we have

$$K_j |q_j\rangle |\psi\rangle = [c_0|0\rangle_j + c_1 \exp(i2\pi\varphi 2^{j-1})|1\rangle_j] \otimes |\psi\rangle$$

where $\mathcal{U}(\tilde{t})|\psi\rangle = \exp(i2\pi\varphi)|\psi\rangle$. The phase φ is what one should read out for the simulation. Treating the product basis for the qubits $|v_1, v_2, \dots, v_n\rangle$, where $v_i = \{0, 1\}$ as an n bit binary number b so that the basis can be denoted as $|b\rangle$, $b = 0, \dots, 2^n - 1$, the inverse quantum Fourier transform (IQFT) performs the mapping

$$\sum_{j=0}^{2^n-1} \frac{\exp(i2\pi j\varphi)}{2^{n/2}} |j\rangle |\psi\rangle \rightarrow |M\rangle |\psi\rangle,$$

where M denotes an n -bit estimate for the phase φ after measurement.

Experimental setup.— A realistic experimental setup for simulation of e-e Coulomb interactions is afforded by trapped

$^{40}\text{Ca}^+$ ions [13]. The number of $^{40}\text{Ca}^+$ ions that can be loaded with present technology ranges from a few to tens of thousands [24], and individual addressing of the ions has been achieved [13]. From the mass ratio between a calcium ion and an electron, the timescale \tilde{t} for this simulator is related to the physical electronic timescale t by $\tilde{t} \approx 1.37 \times 10^{-5}t$.

To simulate an N -electron system the trap is loaded with N ions. The duration for propagation depends on the precision required in the simulation but is limited by the trap decay time, which is around $1\mu\text{s}$ for a radio-frequency ion trap that incorporates an optical cavity [24]. Since the physical electronic time in this example is about 10^5 times the trap evolution time, a relatively long electronic time (~ 0.1 s) can be attained for a trap evolution time that is less than the trap decay time.

To read out the simulation results the ions can be imaged to build a record of position measurements. Then the records can either be mapped to the real electron positions for appropriate initial states, or a Fourier transform can be used to obtain the energy spectrum. Alternatively, a phase-estimation algorithm with a phase precision of n bits can be implemented by sending n qubits initially prepared in the $|0\rangle$ state through Hadamard gates, which is also realizable using ion traps [4, 25]. This readout procedure is capable of high precision since the realization IQFT can be scalable in a semi-classical way [26–28].

Conclusion.— We have proposed a dimensionality-agnostic quantum simulation of the Coulomb interactions in an electron gas by using ion traps loaded with positive ions. The disparity between the masses of electrons and ions, as well as the different charges that the ions may carry, preclude a direct simulation. However, we have shown through a dilatation transform that the propagator of the electron gas at time t gives a spectrum that is mapped one-to-one to the spectrum of the ion trap at a rescaled time \tilde{t} , with the scaling factor between \tilde{t} and t specified completely by the mass of the ion and its degree of ionization. An imaging on the ions can be used to build a measurement record of their positions, which is mapped to the measurement record for electron positions, and a Fourier transform yields the energy spectrum. As a concrete example we have illustrated the experimental setup for this approach using $^{40}\text{Ca}^+$ ions, for which we find that the constraint set by trap decay time should permit electron propagation for as long as ~ 0.1 seconds to be studied.

When only the energy spectrum is required, no additional complexity overhead is added in that we do not need to simulate the dilatation operation on the trapped ions explicitly (it is unitary and does not affect the spectrum). If the wave function is also required, only a simple unitary rotation on the initial state is necessary. Moreover, because of the rescaling of time the runtime of the simulator is much shorter than the timescale for evolution of the electron gas, minimizing the susceptibility of the quantum simulator to external noise and decoherence.

Straightforward extension of this proposal can incorporate different geometries of the trapped ions; for example ion chains [14], ion rings [29], and even periodic lattices [30, 31] are feasible. Particularly interesting applications involve

trapped ions loaded in two-dimensional honeycomb lattices. This would permit emulation of electrons in graphene-like structures, allowing massless Dirac quasiparticles and associated topological phases to be studied [32].

This technique can be extended to many other interesting systems to solve the problem of scale difference between the kinetic and position-dependent terms or, more generally, the problem of terms having different powers of momentum and position dependence.

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